

2-amino-3-(4-chlorophenyl)sulfonylpropanoic acid

5445-04-5 | DTXSID30396827

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 7.20e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.39e-01

Confidence level: 6.74e-01

Nearest Neighbors from the Training Set

Image not found

2-amino-3-(4-chlorophenyl)sulfonylpropanoic acid

Measured: 2.93e-03

Predicted: 7.20e-02

Image not found

Taurocyamine

Measured: 2.33e-01

Predicted: 3.13e-01

Image not found

4-(2-Hydroxyethanesulfonyl)benzene-1-sulfonamide

Measured: 2.49e-02

Predicted: 2.61e-02

Image not found

1H-Imidazole-5-sulfonic acid

Measured: 1.35

Predicted: 7.40e-01

Image not found

1H-Imidazole-2-sulfonic acid

Measured: 8.44e-01

Predicted: 7.41e-01